CFD ANALYSIS OF EMISSIONS FOR A CANDIDATE N+3 COMBUSTOR

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Motivation for Current Work

- NASA N+3 Combustor Development Goals
  - Reduce NOx emissions to 80% below ICAO CAEP6 standards
  - Enhance state-of-the-art for alternate fuels in small core-combustors at higher T_3 (950K) and higher Operation Pressure Ratios (OPR > 50)
  - Leverage N+2 technology achievements of NASA's Environmentally Responsible Aircraft (ERA) project (reduce NOx emissions to 75% below ICAO CAEP6 standards)

Approach for Current Work

- Lean-Direct Injection (LDI) concepts being studied by OEMs and several injector manufacturers
    - Potential to reduce NOx by enhanced mixing, lean burning in primary combustion zones near combustor face
    - All primary air comes into primary combustor zone, no dilution air is used
- Support N+3 Combustor Development with assessment of computational models available in the National Combustion Code (NCC) for a candidate LDI-3 injector design
    - Reacting flow (comparisons of Effective Area, Combustor Temperature, NOx, CO and Unburnt HydroCarbons with LDI-2 experimental data)

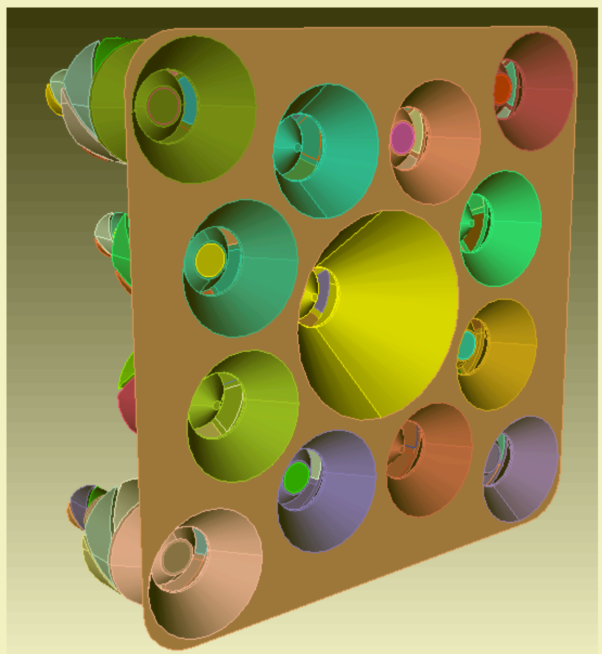
Methods of Current Work

- Derive a candidate 'small core' injector/combustor configuration from N+2 combustor using sets of Airblast and Simplex Injectors split into multiple fuel-stages
- Use updated physical models in the NCC to predict performance and emissions profiles for
  - a candidate LDI-3 geometry configuration at 'medium-power' conditions
  - comparison of RANS (non-reacting and reacting) and TFNS/VLES (non-reacting)

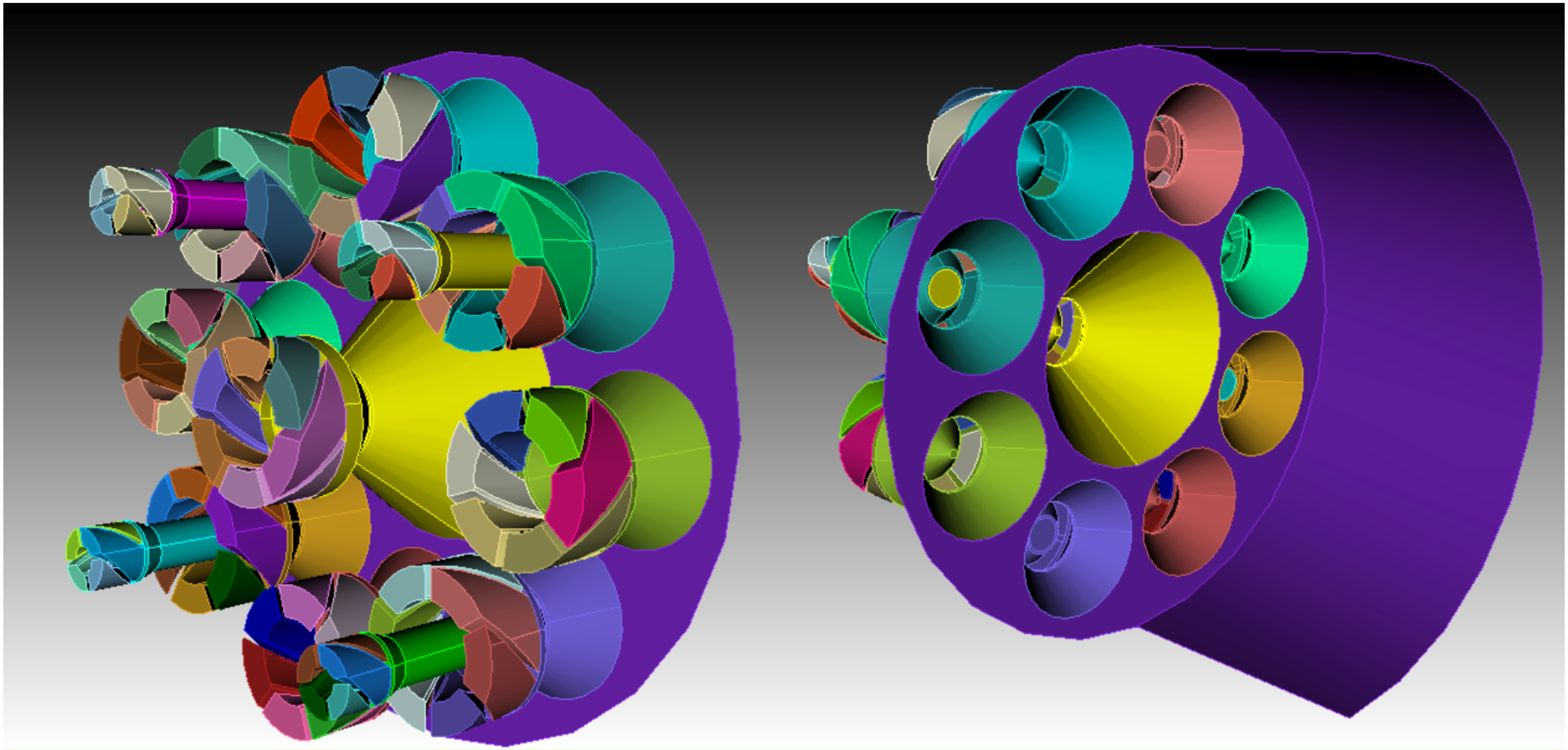
LDI-2 Experimental Configurations

CONFIGURATION	PILOT (Airblast) (OAS/IAS)	MAIN 1 (Simplex)	MAIN 2 (AirBlast) (OAS/IAS)	MAIN 3 (AirBlast) (OAS/IAS)
5Element Recess Config9	57CCW / 57CW	45CW	45CCW / 45CW	45CCW / 45CW
‘Flat Dome’ Config10	Simplex 55CCW	45CCW	45CW / 45CW	45CW / 45CW

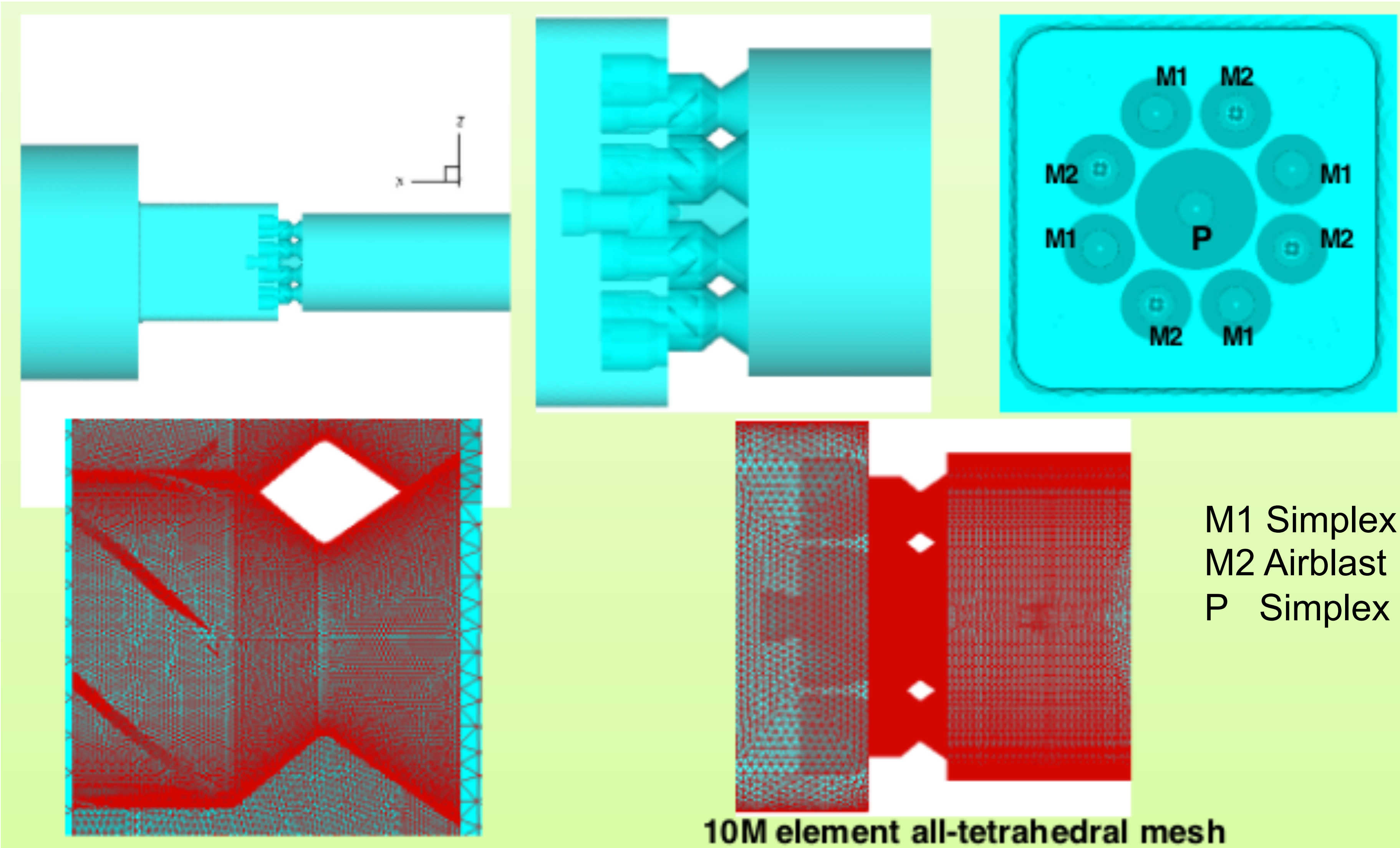
‘Baseline” or ‘Flat Dome’ – Exit plane of the venturi for all thirteen injectors is flush with the main combustor dome
- Single configuration computed with the NCC, compared with NASA GRC data



LDI-3 Candidate (derived from LDI-2)



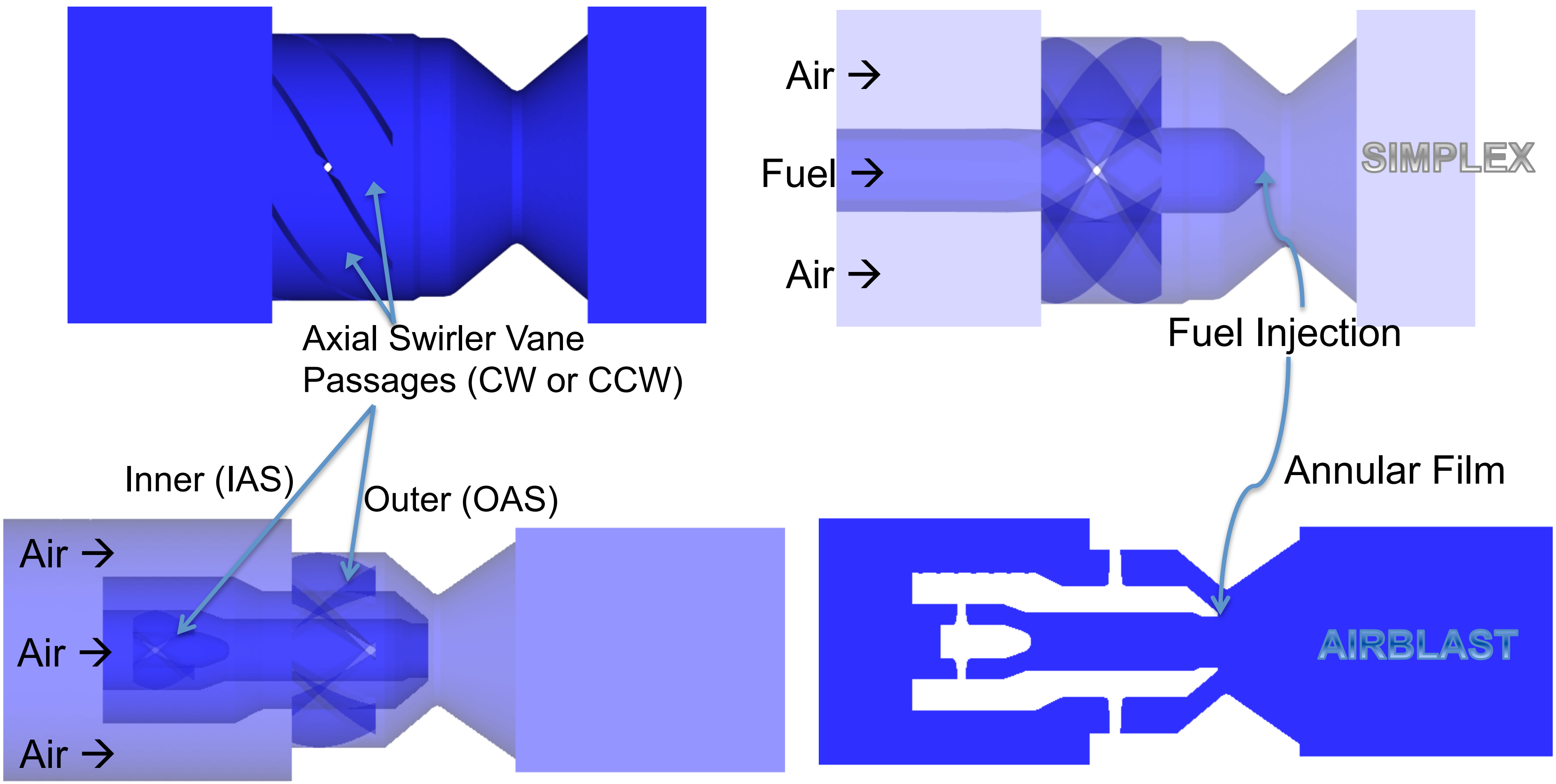
Typical Geometry for WFST LDI-3 Array



Overview of LDI-3 Injection Elements

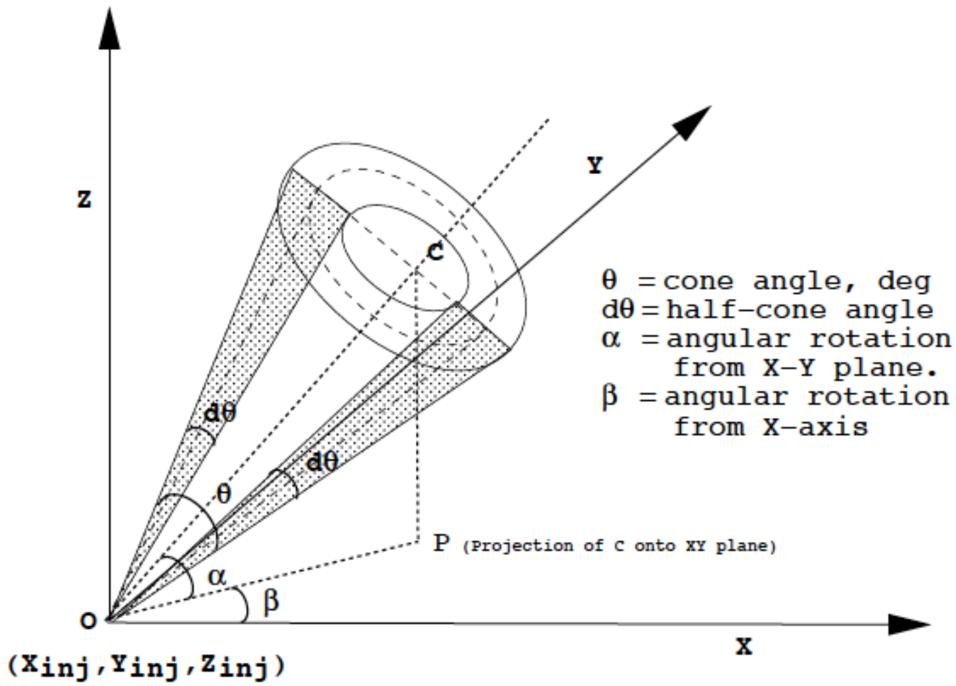
Axial-Bladed-Swirlers with Converging-Diverging Venturi

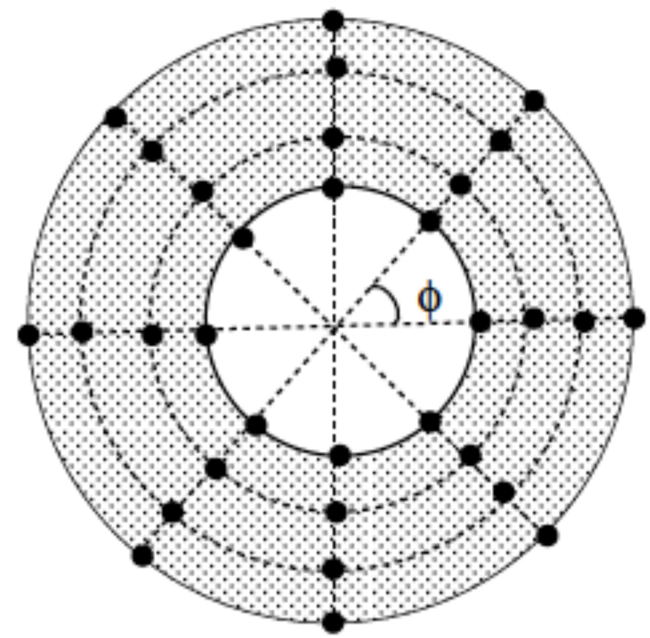
Simplex or Airblast Fuel Nozzle



Various combinations of Simplex and Airblast Elements can be used to form an ARRAY of injectors to achieve operability, efficiency and emissions targets

Spray Initialization for Simplex Injectors





Simplex: θ=60^o $d\theta$=10^o α=0^o β=0^o
60^o 'hollow' cone of 10^o thickness

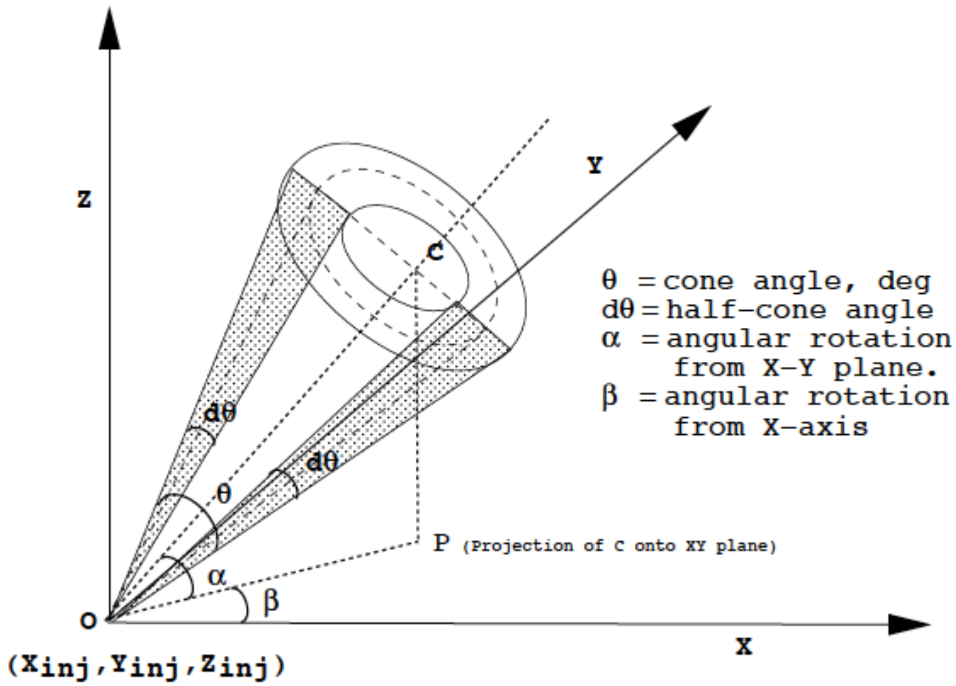
- 32 'streams' per injector
- 10 particle groups per stream
- Injection location and velocity can be varied stochastically as computations proceed

$$\frac{dn}{n} = 4.21x10^6 \left[\frac{d}{d_{32}}\right]^{3.5} e^{-16.98\left(\frac{d}{d_{32}}\right)^{0.4}} \frac{dd}{d_{32}}$$

sauter mean dia = d_{32} < 10μm ; dd=0.2μm
number of droplet groups = 8
dn = number of droplets in the size range *d* and *d + dd*

Y. El Banhawy and J.H.Whitelaw, Calculation of the Flow Properties of a Confined Kerosene-Spray Flame, AIAA J., Vol. 18, pp. 1503-1510, 1980

Spray Initialization for Airblast Injectors



Airblast : $\theta=10^o$ $d\theta=0^o$ $\alpha=0^o$ $\beta=0^o$
10^o ‘**solid**’ cone

- **Airblast ‘film injection’ modeled with 8 or 16 discrete holes for each injector**
- 8 ‘streams’ per discrete hole
- 10 particle groups per stream
- Injection location and velocity can be varied stochastically as computations proceed

M.S. Raju, LSPRAY-IV: A Lagrangian Spray Module, NASA CR-2012-217294

Reduced Mechanism for Jet-A Surrogate

- 14-species,18-step finite-rate chemistry model (Ajmani et al AIAA 2010-1515)
- Jet-A surrogate chemistry, mixture of decane (73%), benzene(18%), hexane(9%)
- Adiabatic flame temperature, flame-speed, ignition-delay matched with shock-tube data
- **allows for in-situ, coupled, computation of emissions (NOx, CO)**

14 Species
18 Steps

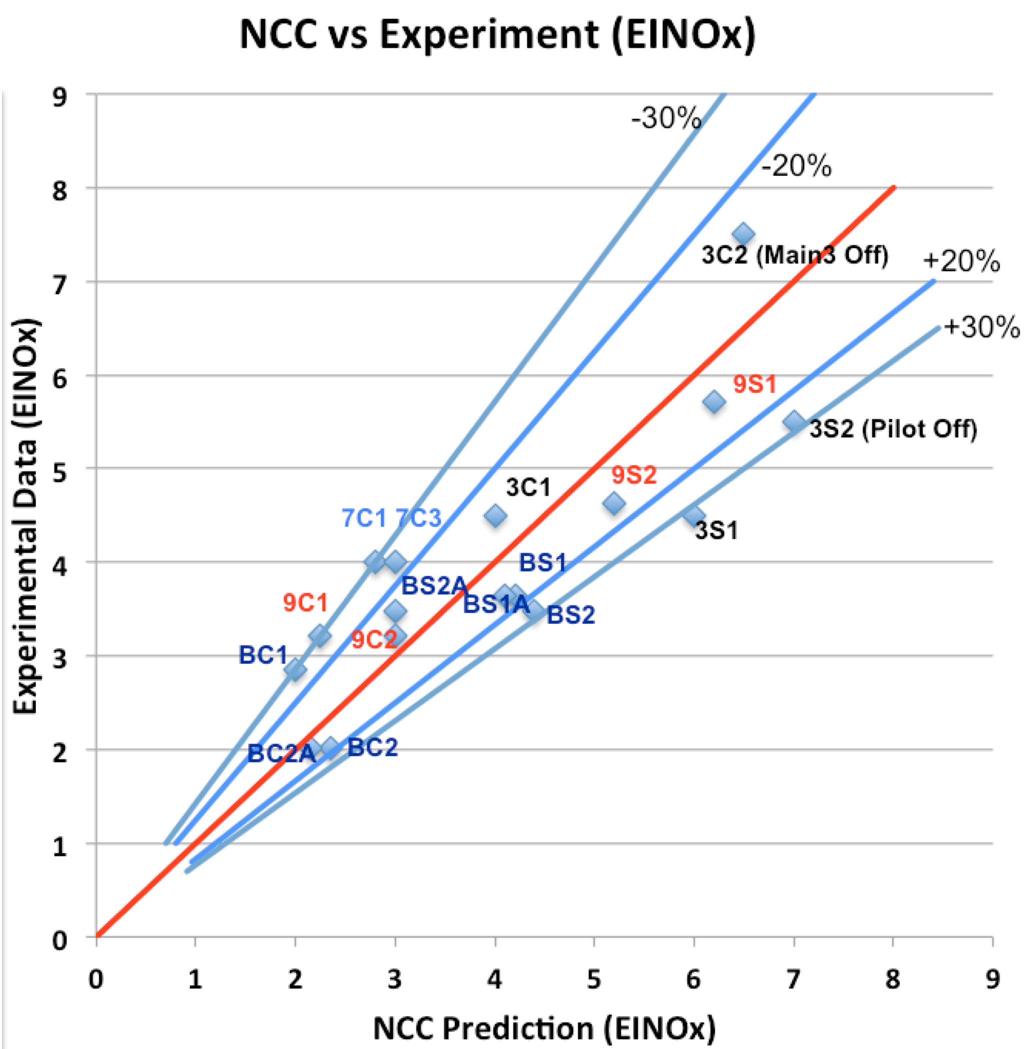
No.	Reaction	A	n	E
1	c11h21 + o2 => 11ch + 10h + o2	1.00E+12	0.00	3.10E+04
	forward /c11h21 0.8/			
	forward / o2 0.8/			
2	ch + o2 => co + oh	2.00E+15	0.00	3.00E+03
3	ch + o => co + h	3.00E+12	1.00	0.00E+00
4	h2 + o2 <=> h2o + o	3.98E+11	1.00	4.80E+04
5	h2 + o <=> h + oh	3.00E+14	0.00	6.00E+03
6	h + o2 <=> o + oh	4.00E+14	0.00	1.80E+04
7	h2o + o2 <=> 2o + h2o	3.17E+12	2.00	1.12E+05
8	co + oh <=> co2 + h	5.51E+07	1.27	-7.58E+02
9	co + h2o <=> co2 + h2	5.50E+04	1.28	-1.00E+03
10	co + h2 + o2 <=> co2 + h2o	1.60E+14	1.60	1.80E+04
11	n + no <=> n2 + o	3.00E+12	0.30	0.00E+00
12	n + o2 <=> no + o	6.40E+09	1.00	3.17E+03
13	n + oh <=> no + h	6.30E+11	0.50	0.00E+00
14	n + n + m <=> n2 + m	2.80E+17	-0.75	0.00E+00
15	h + n2o <=> n2 + oh	3.50E+14	0.00	7.55E+02
16	n2 + o2 + o <=> n2o + o2	1.00E+15	0.00	3.02E+02
17	n2o + o <=> 2no	1.50E+15	0.00	3.90E+04
18	n2o + m <=> n2 + o + m	1.16E+15	0.00	3.32E+04

Use **A** (pre-exponential factor), **n** (temperature exponent) and **E** (activation energy, cal/mol) to compute the Arrhenius rate coefficient, $\mathbf{k = A(T/T_0)^n}\ e^{(-E/RT)}$, for a given temperature, **T** (K). **R** = universal gas constant, $\mathbf{T_0}$ (K) is a reference temperature.

Typical Staged NCC Computational Procedure

- Non-reacting CFD solution
  - k-ε, variable Cμ, non-linear, cubic, with pressure-gradient effect and wall functions
  - Inlet BC: specify mass-flow rate, static temperature ; Exit BC: specify static-pressure ; All walls treated as adiabatic walls
- Reacting Flow Solution
  - Use ignition sources in region downstream of venturi-exit – ignition sources turned off once temperature in any element in mesh reaches 1600K
  - Use spray parameters (SMD, velocity) provided by Woodward FST
  - Lagrangian spray model (spray angle, θ = 60, spray thickness angle dθ = 10, 32 streams, 8 droplet groups, stochastic model, no secondary breakup)
  - Finite-rate chemistry models – 14species, 18 steps (direct NO computation)
    - Account for prompt, thermal, N2O NOx pathways

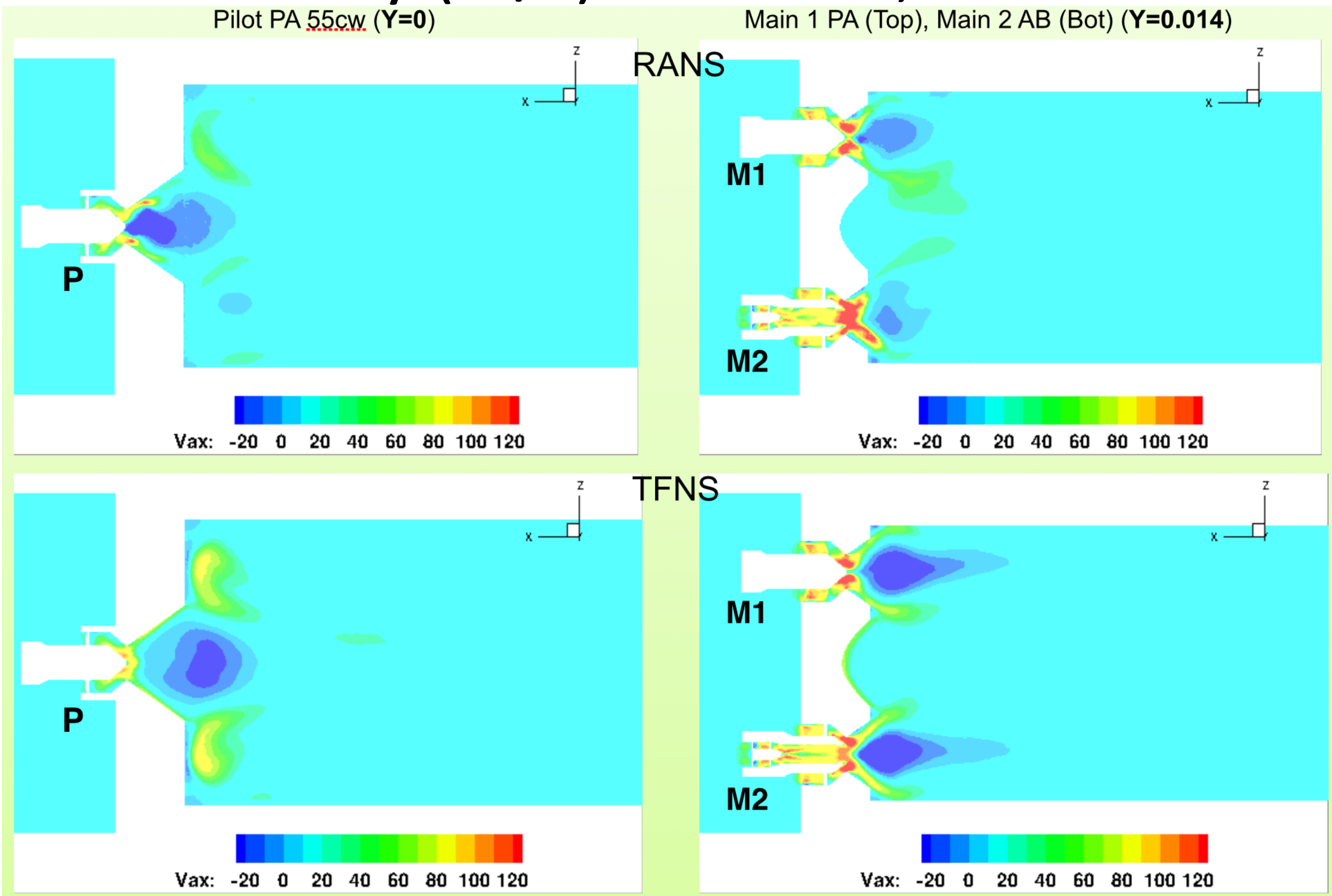
Validation of NCC RANS for LDI-2 Configurations Predicted vs Experimental EINOx Data



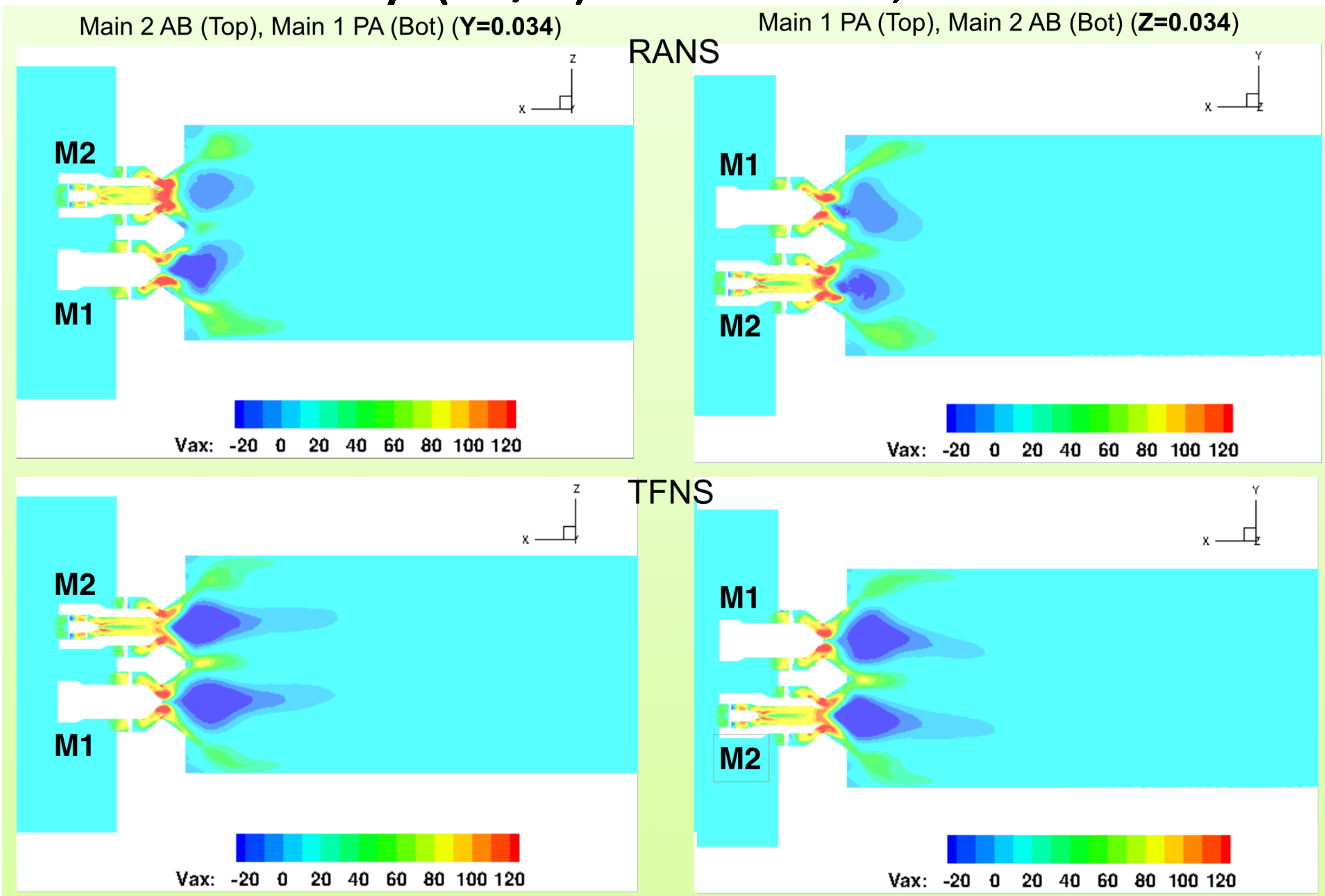
RANS vs TFNS/VLES

Non-Reacting Flow

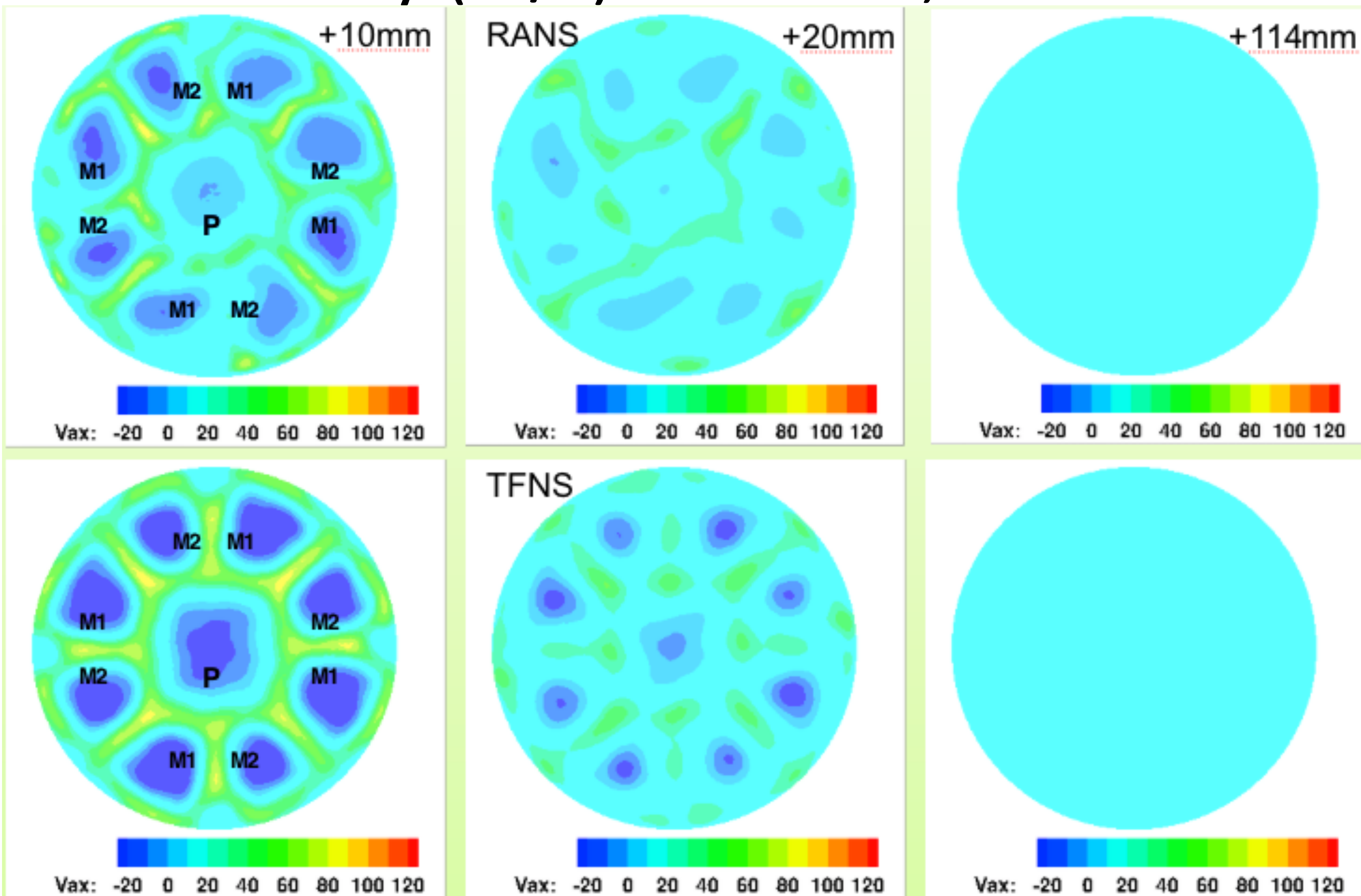
Axial Velocity (m/s) Contours, RANS vs TFNS



Axial Velocity (m/s) Contours, RANS vs TFNS



Axial Velocity (m/s) Contours, RANS vs TFNS



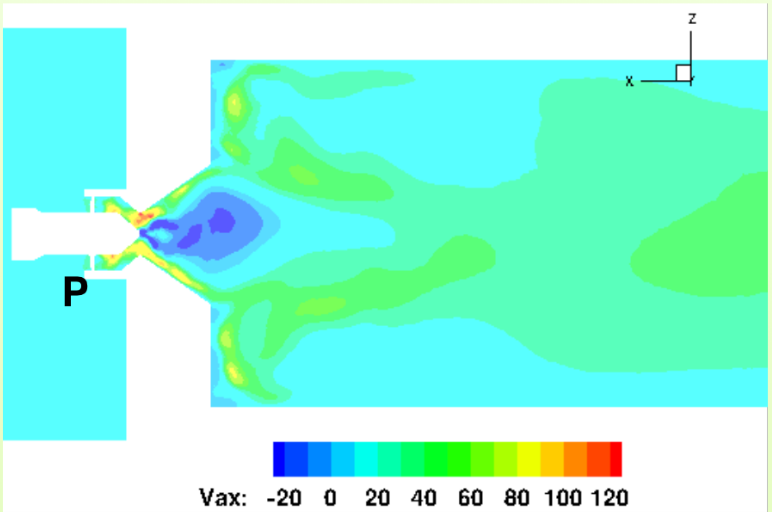
RANS Reacting Flow CFD

Axial Velocity (m/s) Contours, RANS Reacting

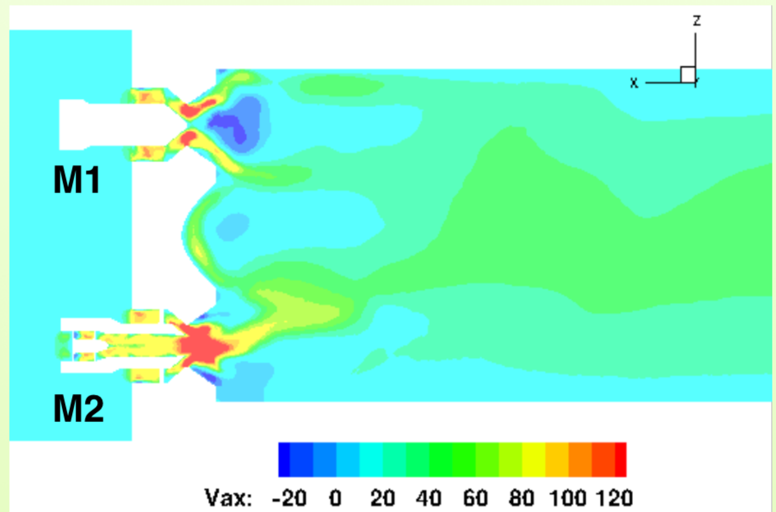
Transverse Cross Sections

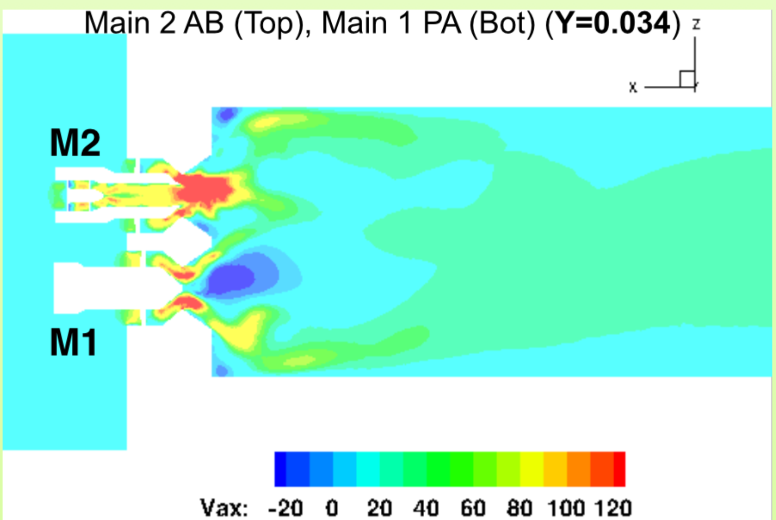
RANS

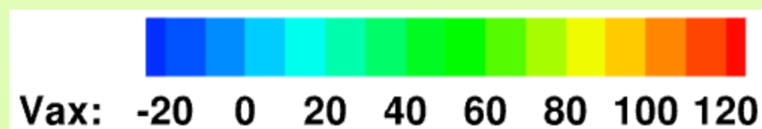
Pilot PA 55cw (**Y=0**)



Main 1 PA (Top), Main 2 AB (Bot) (**Y=0.014**)







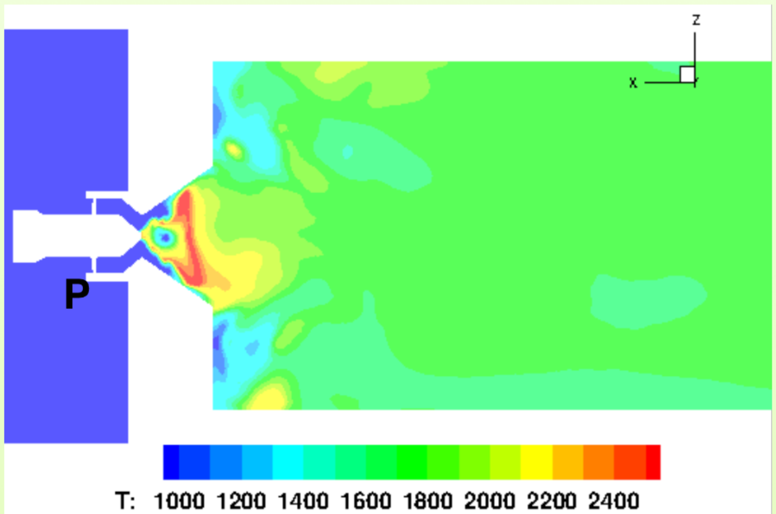
AC_d	AC_d (NCC)	CFD %Error
(in^2)	(in^2)	
1.40	1.39	-0.07%

Temperature (K) Contours, RANS Reacting

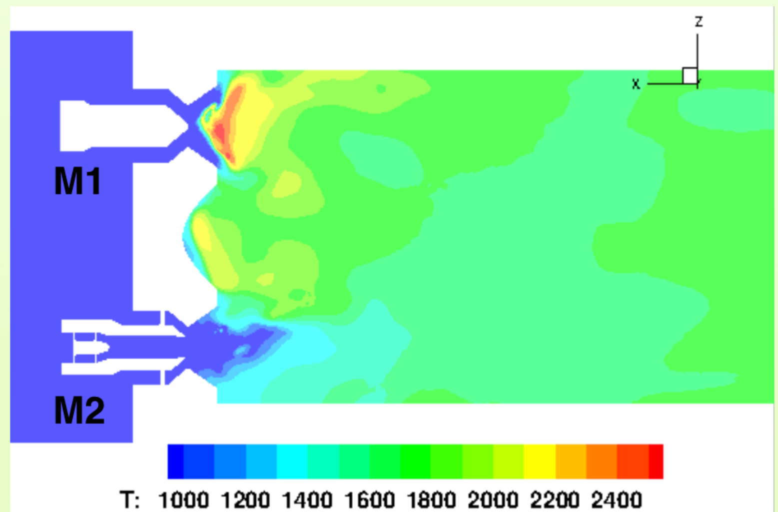
Transverse Cross Sections

RANS

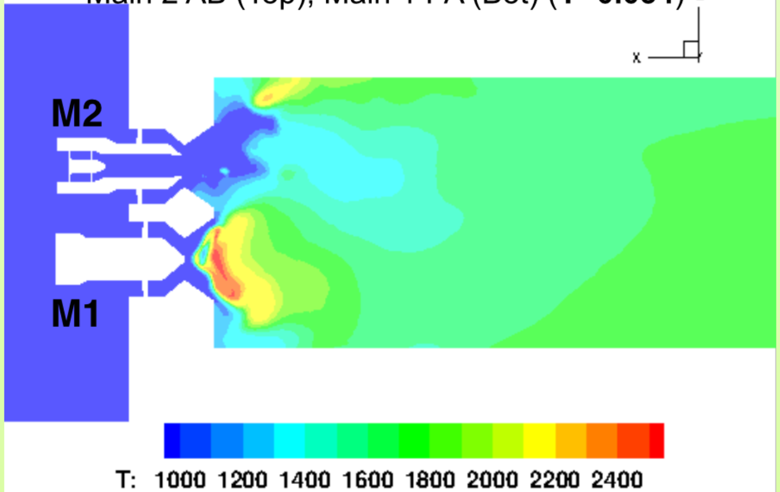
Pilot PA 55cw (**Y=0**)

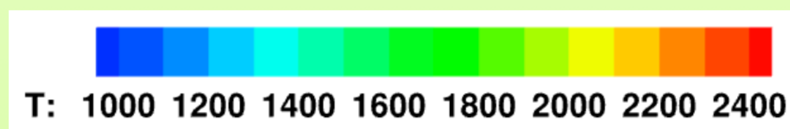


Main 1 PA (Top), Main 2 AB (Bot) (**Y=0.014**)



Main 2 AB (Top), Main 1 PA (Bot) (**Y=0.034**)

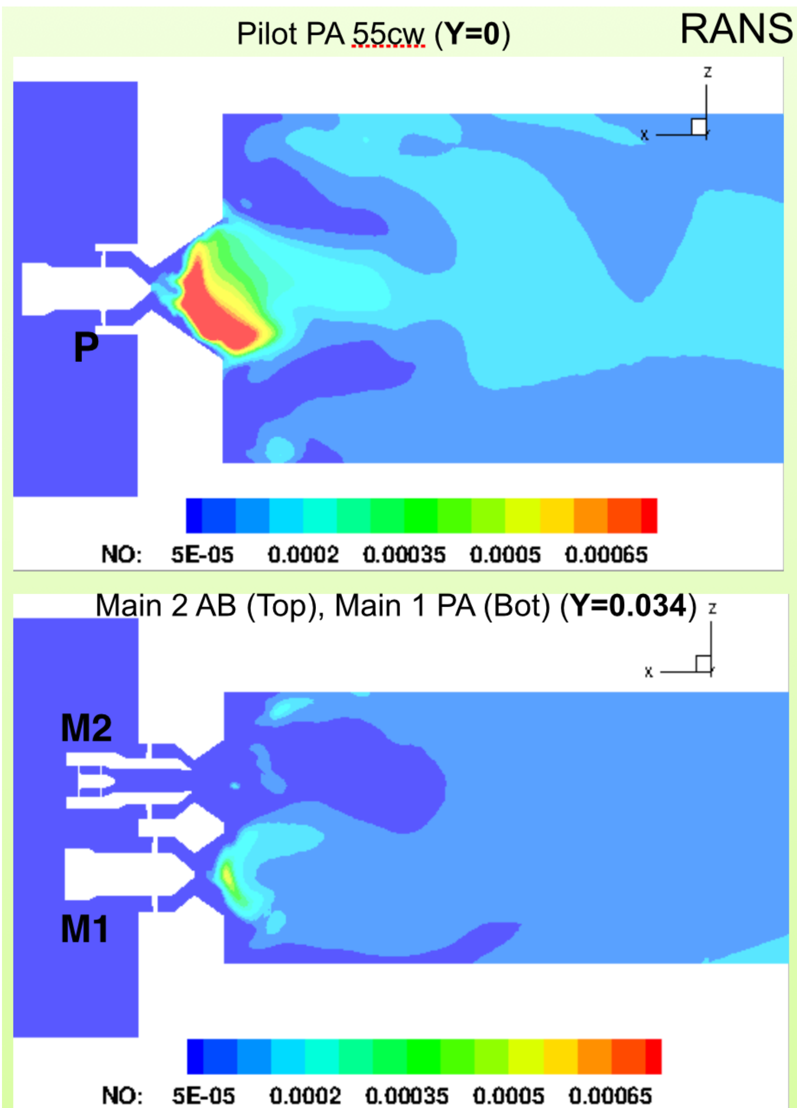


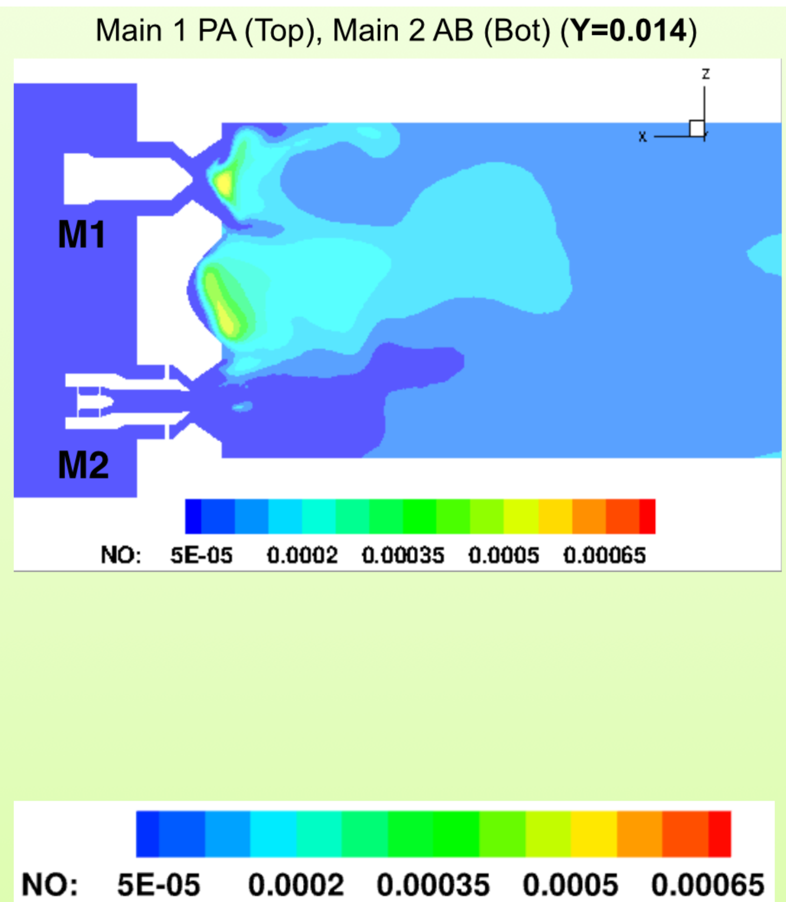


T4 (CEA)	T4 (NCC)	CFD % Error
(K)	(K)	(K)
1723	1710	-0.8%

NO mass-fraction Contours, RANS Reacting

Transverse Cross Sections

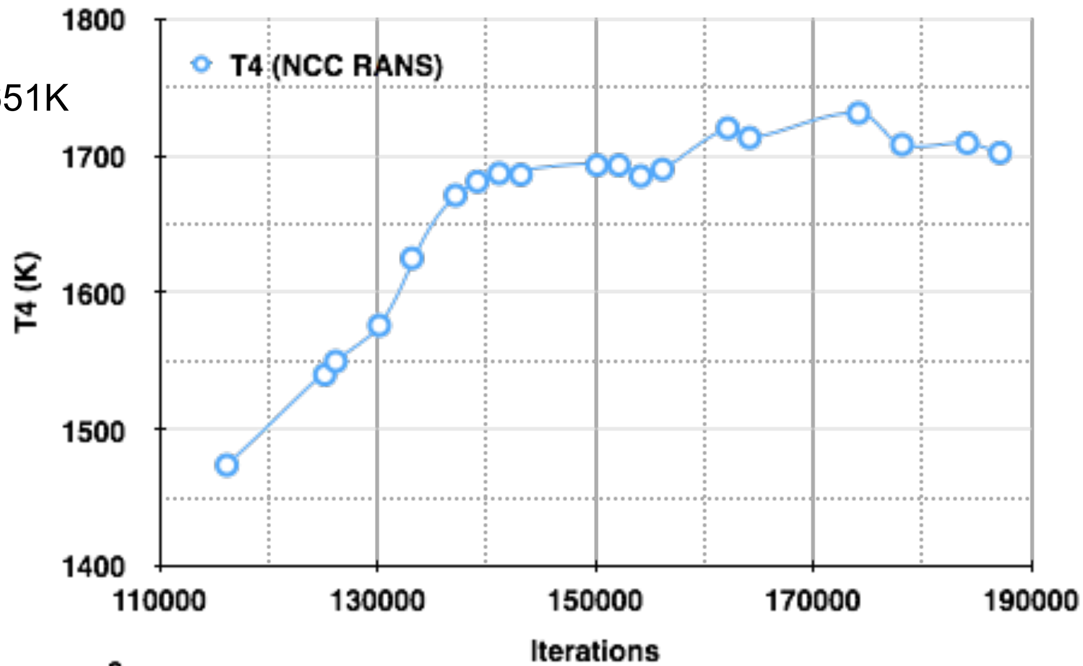




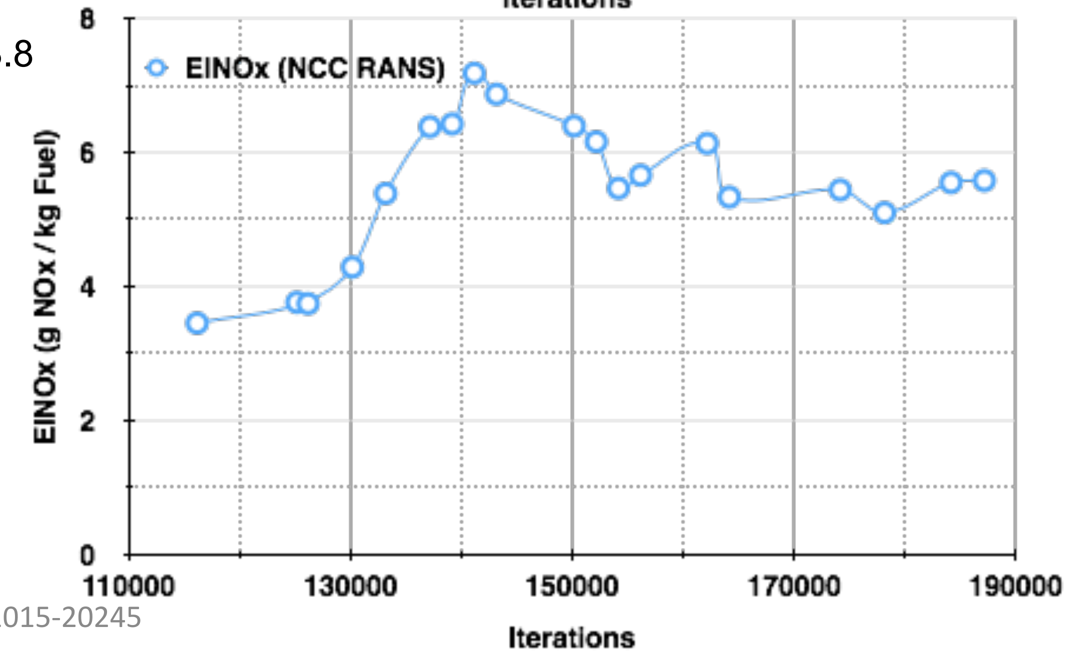
EINO (Correlation)	EINO (NCC)	CFD %Error
g/kg of Fuel	g/kg of Fuel	
6.27	6.6	+5.3%

Typical Convergence History

T4 (CEA)=1651K



EINOx (Expt)=3.8

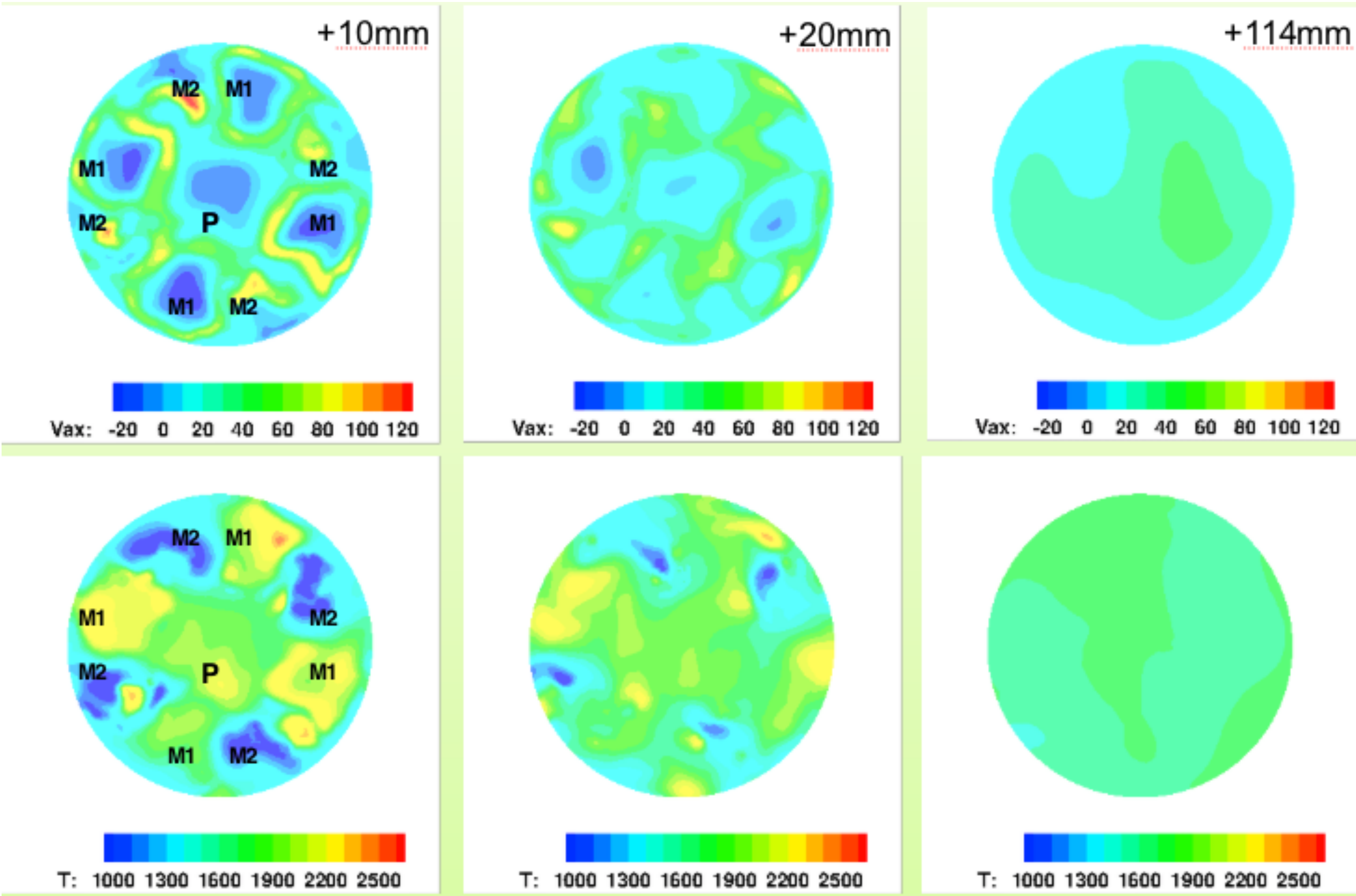


Medium Power Case

Mass-weighted average of T4 and EINOx across exit plane of CFD Domain

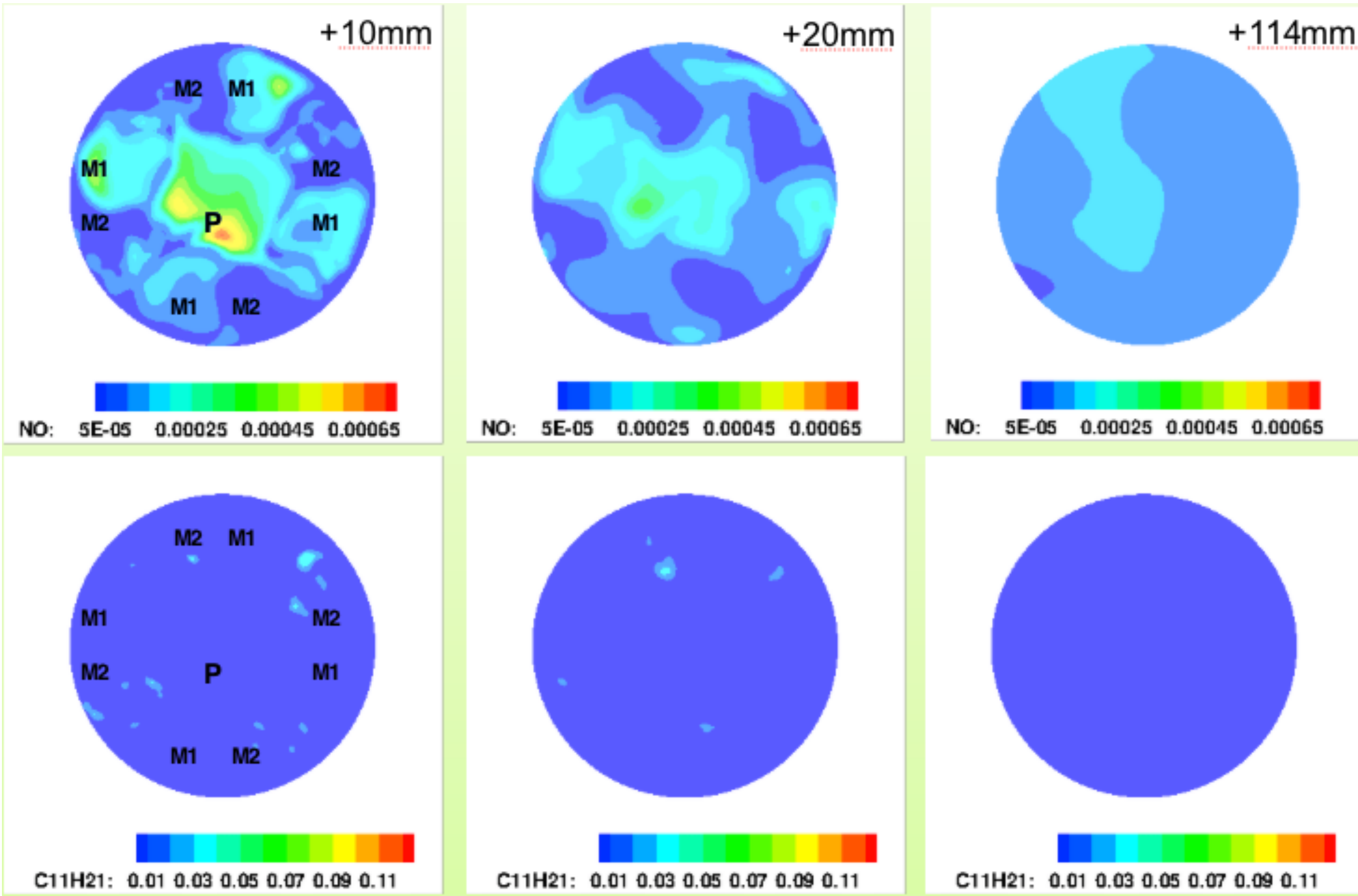
Axial Velocity (m/s), Temperature (K) RANS Reacting

Axial Cross Sections



NO mass-fraction, UHC mass-fraction RANS Reacting

Axial Cross Sections



RANS Reacting Flow Summary

LDI-3 'Candidate' – Medium Power Conditions
Summary EINOx, Exit Temperature, T_4 (K)

	T3	FAR	EINOx (Expt)	EINOx (NCC)	T4 (Expt)	T4 (NCC)
	(K)		(g /kg Fuel)	(g /kg Fuel)	(K)	(K)
N+3	950	0.0234	6.27	6.6	1710	1723
N+2	810	0.0261	3.8	5.4	1651	1698

- Average Exit temperature (T4) predicted by NCC matches experimental data to within 1% for candidate N+3 medium-power conditions.
- EINOx prediction by NCC (6.6) is within 5% error of extrapolated data (6.27) from correlation equation of Tacina et. al
  - [Tacina 2014] Tacina, K.M., Chang, C., He, Z.J., Mongia, H.C., Dam, B., and Lee, P., "A Second Generation Swirl-Venturi Lean Direct Injection Combustion Concept," AIAA Paper 2014-3434, AIAA Propulsion and Energy Conference, Cleveland, OH, July 2014.
- EINOx extrapolation for N+3 is from Glenn Research Center flame-tube data for N+2 configuration

$EINOx = p_3^{0.5}\, e^{T_3/230}\, (Dp/p)^{-0.6}\, (a_1 f_1^{b1} + a_2 f_2^{b2} + a_3 f_3^{b3})$

a_1=0.0081, b_1=0.29, a_2=0.35, b_2=7.15, a_3=0.369, b_3=7.37

f_1, f_2, f_3 are the equivalence ratios for the P, M1, M2/M3 stages.

Lessons Learned and Future Work

- RANS solutions may be very useful as a *first-cut* to narrow the design matrix at medium-power conditions evaluated here; a stepping-stone to time-accurate TFNS/VLES computations.
- TFNS Reacting Flow is prohibitively expensive for design iterations in preliminary design phase, particularly with *in-situ* emissions computations
- NCC RANS predicts EINOx values to within 5% of extrapolated data for medium-power N+3 conditions. Additional CFD predictions of N+3 performance needed for low- and high-power conditions .
- Future work: Evaluate N+3 configuration with reduced-kinetics mechanism *optimized* for emissions
    - AIAA-2014-3662. A Reduced Mechanism for Combustion of Jet-A in LDI Combustor CFD Calculations *Kumud Ajmani; Krishna Kundu; Shaye J. Yungster*

Acknowledgements

- Subsonic Fixed Wing (SFW) Project at NASA GRC
- Environmentally Responsible Aircraft (ERA) Project at NASA GRC

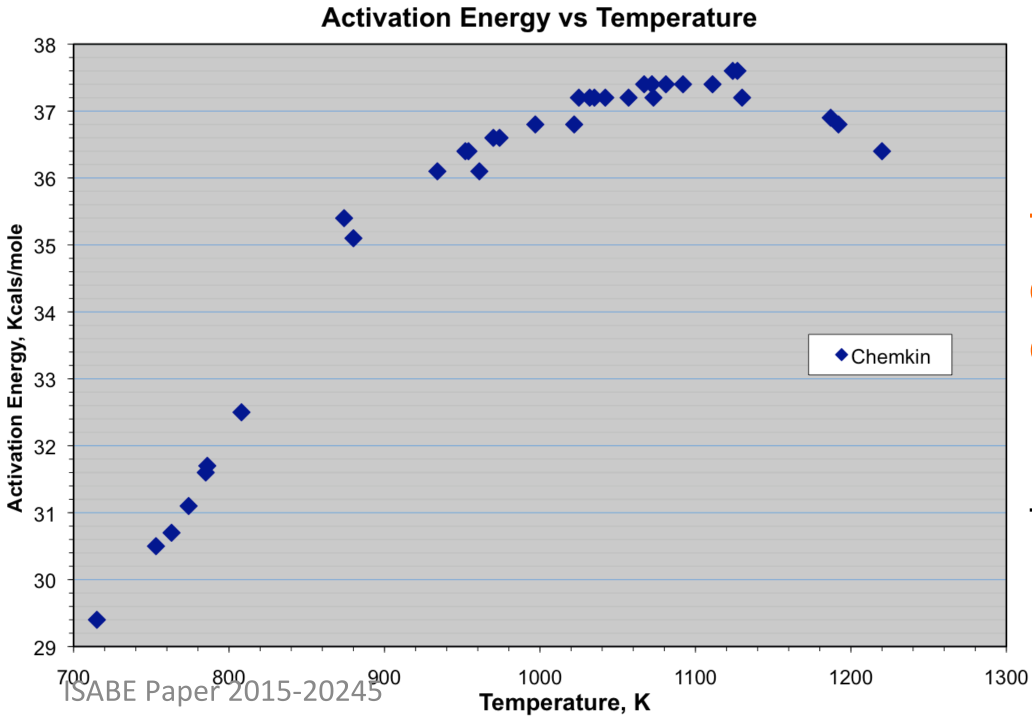
Backup Slides

Summary of National Combustion Code (NCC)

- Two-dimensional axi-symmetric or full three-dimensional computations
- Most unstructured and structured mesh element types can be computed
- Finite-Volume solutions of Time-dependent, Navier-Stokes equations
- Dual time-stepping for 2nd order time-accuracy with 4-stage Runge-Kutta scheme
- 2-equation, k-ε turbulence models (non-linear, low-Re or wall-functions) ("Generalized Wall Function for Complex Turbulent Flows,", T.-H. Shih, L.A. Povinelli, K.- H. Chen, N.-S. Liu, NASA TM 2000-209936.)
- Lagrangian spray-modeling with primary/secondary breakup and atomization options, multi-component fuels ("LSPRAY-IV: A Lagrangian Spray Module", M. S. Raju, NASA CR-2012-217294, Glenn Research Center, Cleveland, OH.)
- Reduced-kinetics, Finite-rate chemistry models of varying complexity available for various fuels
- Turbulence-chemistry interaction modeled with one of several different approaches
- RANS time-integration and/or VLES with Time-Filtered Navier-Stokes (TFNS) approach

Chemistry Mechanism

- 14-species,18-step finite-rate chemistry model (Ajmani et al AIAA 2010-1515)
- Jet-A surrogate chemistry, mixture of decane (73%), benzene(18%), hexane(9%)
- Adiabatic flame temperature, flame-speed, ignition-delay matched w/experimental shock-tube data
- Iterate with CHEMKIN to find activation energy for fuel breakup step which produces a close match between computed ignition delay and experimental ignition delay for a particular ϕ , P, initial temp. (T)



Temperature dependent activation energy as Jet-A is not a single compound

For CFD code, adjust activation energy in breakup step based on initial temperature